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Translation #1057

ELECTRONIC CHEMISTRY. - $Mg^{2+}$ and $Ca^{2+}$ activators in the cycle of chemical reactions of muscular contraction. Note (*) of Madame Audree Goudot, presented by M. Louis de Broglie.
Compt. rend. 254:3096-3098, 1962.

Chemical analysis of muscle fibers shows that they contain the following main aminated acids: Lysin, arginin, alanin and a certain number of others which have an alanin termination.

On the other hand the organic phosphorus used in vivo is the phosphogene (creatine-P). The "fuel" is provided by glucoses and phosphates. Furthermore, acetylcholine intervenes as an excitant originating in the nervous system. Finally, in the fundamental process $Mg^{2+}$ and $Ca^{2+}$ are indispensable.

1. Phosphogene utilization. - A preceding study has shown that in a magnesium complex the rupture between the phosphate connection of phosphogene has roughly the same energy as for adenosinetriphosphate (ATP). It seems therefore that phosphogene is specifically utilized in muscular contraction because of the chemical nature of creatine. Therefore, if ATP is the intermediary of the transphosphorylation, the specific reaction must occur between proteins. Furthermore, in the contraction, two thirds of the transformed substances are sugars and phosphates, but one third is made up of albuminoid matters.

The following relation can be drawn between creatin, arginin and alanin: $Creatin+Alanin^{M2}= Argin+Acetyl$.

It is therefore important to know whether, through the intermediary of phosphorylation, the indispensable metal cations can achieve such chemical reaction. The calculation of the repartition of charges makes it possible to foresee between which neighboring atoms, which have become strongly positive,

a connection rupture can occur.

1° Creatin-P-$M^{2+}$ -alanin.

| Alanine | $M^{2+}$. | O. | CO. | C. | $NH_2$. | $CH_3$. |
|---|---|---|---|---|---|---|
| $Mg^{2+}$ ..... | −0,29 | −0,81 | +0,13 | −0,77 | +0,10 | −0,59 |
| $Ca^{2+}$ ..... | −0,08 | −0,93 | +0,09 | −0,80 | +0,30 | +0,53 |

| Créatine | $CO_2$. | $CH_2$. | $NH_2$. | $CH_2$. | $NH_2$. | C. | $NH_2$. |
|---|---|---|---|---|---|---|---|
| $Mg^{2+}$ ..... | −0,72 | +0,77 | +0,21 | −0,20 | +0,40 | +0,08 | +0,45 |
| $Ca^{2+}$ ..... | −0,76 | +0,79 | +0,22 | −0,20 | +0,41 | +0,08 | +0,45 |

a. A rupture can occur between $CH_2$(+0.77 or +0.79) and N(+0.21, +0.22), thus dissociating the acetyl grouping from creatin.

b. A connection may occur between $CH_2$(+0.59, +0.53) of alanin and -$CH_2$(-0.20) of creatin, yielding 1 mol of arginin.

The distribution of charges is roughly the same in the magnesium complex and in the calcium complex.

One must also know whether the reaction is reversible, that is whether the same cations activate the reverse reaction.

2° Arginin-P - $M^{2+}$-acetyl:

| | | Arginine. | | | | | |
|---|---|---|---|---|---|---|---|
| | $M^{2+}$. | O. | CO. | CH. | $NH_2$. | $CH_2$. | $CH_2$. |
| $Mg^{2+}$ ..... | −0,74 | −0,85 | +0,22 | −0,09 | +0,32 | +0,29 | +0,65 |
| $Ca^{2+}$ ..... | −0,05 | −0,94 | +0,10 | −0,09 | +0,48 | +0,31 | +0,62 |

| | Arginine. | | | | Acétyl. | |
|---|---|---|---|---|---|---|
| | $NH_2$. | $NH_2$. | $CH_2$. | $NH_2$. | CO. | $CH_3$. |
| $Mg^{2+}$ ..... | −0,86 | +0,54 | +0,35 | +0,47 | −0,82 | +0,80 |
| $Ca^{2+}$ ..... | −0,82 | +0,41 | +0,08 | +0,48 | −0,80 | +0,82 |

a. Rupture between $CH_2$(+0.29 or +0.31) and $CH_2$(+0.65, +0.62), thus dissociating an alanin molecule from an arginin molecule.

b. For the calcium complex, there can be formation of 1 mol of creatin through connection between -$CH_2$(+0.82) and NH(-0.82).

c. In the magnesium complex a desamination may occur.

2. Lysin-phosphoglyceric acid cycle. - The glycogene being consumed in the course of contraction, it may be suggested that there is a reaction where a phosphoric ester enters (( and where)) by deriving phosphoglyceric acid one has lysin+ phosphoglyceric acid $\overset{M2}{\rightleftharpoons}$ alanin+cholin+carbonyl phosphate. The theoretical study consists in seeing whether $Mg^{2+}$ and $Ca^{2+}$ are activators.

1° Lysin-$M^{2+}$-phosphoglyceric acid.

| | | Lysine. | | | | |
|---|---|---|---|---|---|---|
| | $M^{2+}$. | O. | CO.....$CH_2$. | $CH_2$. | $CH_2$. | |
| $Mg^{+2}$..... | −0,21 | −0,71 | +0,73 | 0,0 | +0,88 | +0,86 |
| $Ca^{2+}$..... | −0,05 | −0,68 | +0,74 | −0,10 | +0,87 | +0,85 |

| | Lysine. | | Phosphoglycéride. | | | | |
|---|---|---|---|---|---|---|---|
| | $CH_2$. | $NH_2$. | $CH_2$. | CHOH. | CO. | O. | P. |
| $Mg^{+2}$..... | +0,88 | −0,65 | −0,77 | +0,94 | +0,84 | −0,82 | +0,83 |
| $Ca^{2+}$..... | +0,87 | −0,65 | −0,87 | +0,94 | +0,83 | −0,91 | +0,83 |

a. For the magnesium complex there is possible rupture between $CH_2$ neutral and $CH_2$(+0.88), dissociating 1 mol of alanin. That is not possible for the calcium complex where $CH_2$ (-0.10) and $CH_2$ (+0.87) neighboring each other.

b. Dissociation between $CH_2$(+0.88), $CH_2$(+0.86, $CH_2$(+0.88) which can yield with $NH_2$(-0.65) $N(CH_3)3$ and formation of choline with $CH_2$(-0.77) and CHOH(+0.94).

c. Probable rupture between CHOLH(+0.94) and CO(+0.84).

It therefore seems that only $Mg^{2+}$ can be activator of this reac ion.

2° Alanin-$M^{2+}$-cholin-carbonyl phosphate.

| | | Alanine. | | Choline. | | |
|---|---|---|---|---|---|---|
| | $M^{2+}$. | O. | CO.....$CH_2$. | $CH_2$. | $CH_2$ | $CH_2$. |
| $Mg^{2+}$..... | −0,20 | −0,74 | +0,83 +0,97 | −0,10 | +0,72 | −0,86 |
| $Ca^{2+}$..... | −0,03 | −0,69 | +0,74 +0,90 | −0,28 | +0,73 | −0,85 |

| | Choline. | | Carbonyl Phosphate | | | |
|---|---|---|---|---|---|---|
| | N. | $CH_2$. | CHOH. | CO. | O. | P. |
| $Mg^{2+}$..... | +0,28 | +0,24 | −0,13 | +0,98 | −0,01 | +0,98 |
| $Ca^{2+}$..... | +0,38 | +0,19 | −0,14 | +0,98 | −0,10 | +0,83 |

a. Possible connection between $CH_2$(+0.97, +0.90) and $CH_3$(-0.1, -0.28) and a rupture between N(+9.28, +0.38) and $CH_2$(+0.24, +0.19). There can thus be formation of 1 mol of lysin.

b. Rupture between CO (neutral, +0.10) thus freeing 1 mol of lactic acid $CH_3$-CHOH-COOH.

In this reaction $Ca^{2+}$ is a better activator than $Mg^{2+}$.

Activation potential. - It represents the difference between the energy of electronic delocalization of the complex metal cation-reaction products and that of the activated complex metal cation-substrates.

In cycle I (phosphogene) this potential is 4.8 kc for the calcium complex and 4 kc for the magnesium complex. In cycle II (phosphoglyceric acid) this potential is 123.15 kc for the magnesium complex and 117.28 for the calcium complex. In each cycle there is an energy of coorelation between the magnesium complex and the calcium complex.

Discussion. - In both cycles the first reaction has $Mg^{2+}$ for activator and the second reaction has $Ca^{2+}$ for activator. It is therefore possible to schematize both types of muscular contraction through two dynamic cycles:

Cycle I (phosphogene) of small coorelation energy $Mg^{2+}/Ca^{2+}$ : 0.8 kc.

Cycle II (photoglyceric acid) whose coorelation energy frees 5.87 kc. In both cycles there is an intermediary alanin remnant which can act as serine or cysteine connection between actin and myosin, according to Weber's representation.

(*) Seance of 16 April 1962.